

beta-Caryophyllene
87-44-5 | DTXSID8024739

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 9550 L/kg

Global applicability domain: Inside

Local applicability domain index: 3.87e-01

Confidence level: 7.70e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Pendimethalin</div> <div>Measured: 5010</div> <div>Predicted: 4980</div>	<div>Image not found</div> <div>9-Methylanthracene</div> <div>Measured: 64600</div> <div>Predicted: 29700</div>	<div>Image not found</div> <div>Dinoseb</div> <div>Measured: 501</div> <div>Predicted: 296</div>
<div>Image not found</div> <div>Anthracene</div> <div>Measured: 20400</div> <div>Predicted: 19600</div>	<div>Image not found</div> <div>Phenanthrene</div> <div>Measured: 22400</div> <div>Predicted: 19900</div>	